

Model Atmospheres for Cool Massive Stars

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Abstract. In this review given at the Hot and Cool: Bridging Gaps in Massive Star Evolution conference, I present the state of the art in red supergiant star atmosphere modelling. The last generation of hydrostatic 1D LTE MARCS models publicly released in 2008 have allowed great achievements in the past years, like the calibration of effective temperature scales. I rapidly describe this release, and then I discuss in some length the impact of the opacity sampling approximation on the thermal structure of models and on their emergent spectra. I also insist on limitations inherent to these models. Estimates of collisional and radiative time scales for electronic transitions in e.g. TiO suggest that non-LTE effects are important, and should be further investigated. Classical 1D models are not capable either to provide the large and non-gaussian velocity fields we know exist in red supergiants atmospheres. I therefore also present current efforts in 3D radiative hydrodynamical simulation of RSGs. I show that line profiles and shifts are predicted by these simulations, without the need for fudge micro- and macroturbulence velocities. This is a great progress, although line depths and widths are slightly too shallow. This is probably caused by the simplified grey radiative transfer used in these heavy simulations. Future non-grey 3D simulations should provide a better fit to observations in terms of line strengths and widths.

1. Classical Model Atmospheres

Model stellar atmospheres constitute the basis on which we interpret stellar spectra. Our ability to produce "good" models including the necessary physical approximations and input data directly impacts the quality and reliability of the parameters we extract from observations: T_{eff} , chemical abundances, etc. We know red supergiant (RSG) atmospheres are subject to strong convective motions, resulting in temperature inhomogeneities, and velocity fields. Particle densities are low and non-LTE effects are expected (see below). Despite this complexity, simple one-dimensional, hydrostatic, LTE models have been constructed, and used to study RSGs with success. I start by presenting the current MARCS generation of such models, detailing some aspects linked to the opacity sampling approximation. I then show how velocity fields affect the spectra, and discuss possible non-LTE effects on molecules. Finally I present current efforts in hydrodynamical modelling, with encouraging results, but with their own limitations, hopefully alleviated in the near future.

1.1. MARCS 2008

The MARCS model atmosphere code has been in use since the mid-70's. The official birth certificate of MARCS, a code for Model Atmospheres in Radiative

and Convective Scheme, is Gustafsson et al. (1975). It allowed the computation of hydrostatic, plane-parallel (PP), line-blanketed atmospheres, with convection included following Henyey, Vardya, & Bodenheimer (1965) recipe for MLT, and line opacity treated in the form of Opacity Distribution Functions (ODF). Many updates were implemented since then, and a major release was published recently (Gustafsson et al. 2008). MARCS 2008 is characterised by, e.g., new opacities for H_2O , atomic collisional line broadening included using the description of Anstee & O'Mara (1995), and hydrogen lines modelled using a code by Barklem, described in Barklem & Piskunov (2003). About 108 000 opacity sampling points are used (see next section). All atomic and molecular line opacities were reviewed, as well as continuous opacities. More than half a billion lines are included, e.g. TiO , ZrO , VO , CO , CN , MgH , just to list a few. Full details are provided in Gustafsson et al. (2008), that also relates some of the historical background, and discusses in depth the physical assumptions, numerical methods, and physical data used. Additional historical details are provided in Plez (2008). About 30 000 models have been computed at the time I am writing these lines in early 2009. A standard grid is available on the web (marcs.astro.uu.se).

1.2. Sampling of Opacities, Model Thermal Structure, and Fluxes

In MARCS, as well as in most modern model atmosphere codes, the opacity is treated with the opacity sampling (OS) approximation. This is a Monte-Carlo evaluation of the radiation field using a set of wavelengths where the opacities, and monochromatic contributions to the intensities, flux, radiation pressure, and all radiation field characteristics are calculated. A simple summation over wavelength gives the wavelength integrated quantities. In principle, if the number of wavelengths is large enough, this approach is safe. There are however two questions to be investigated: (i) how many OS points are needed for a given convergence of the model (e.g. temperature corrections $\Delta T < 1\text{K}$)? (ii) how well is the spectrum represented, e.g. to compute synthetic photometry or do spectral classification? This was discussed by Plez (2008), and I will only recall here what concerns more specifically RSGs. In these cool star atmospheres the dominant opacity is that of molecules: CO , TiO , H_2O . The latter two have a very dense spectrum with lines mostly blended with one another. This makes the OS approximation very well functioning. On the contrary CO , in the H, K and L bands has fewer, well separated lines. At a resolution of 20 000, the wavelength sampling does not represent evenly strong and weak lines, and the continuum. This is demonstrated by statistics on ensembles of models computed with various samplings: the nominal $R = \lambda/\Delta\lambda = 20000$, and models with reduced $R = 6700$, $R = 2000$, and $R = 670$, for a wavelength range between 900\AA and $20\mu\text{m}$. I computed the standard deviation to the reference high resolution model of models with sparser sampling. For cool models representative of RSGs, the deviations in the temperature structure are very small: always less than about 10K at the lowest resolution, and less than 3K for the $R = 6700$ models. This is because the opacity that matters for the thermal structure of these star atmospheres (TiO and H_2O) is statistically well taken into account even at low resolution. This is not the case for the rendering of the spectrum. Under-sampling causes local errors in fluxes. For RSGs, and after smoothing to $R = 200$, errors amount to about 10% in the blue-UV, and about 5% in the IR

CO bands, for a sampling at $R = 6700$. Sampled spectral energy distributions (SEDs) should not be compared to observed spectra at medium-high resolution. Even when the SEDs are degraded to low resolution (a few 100), systematic errors remain at a level of several % for an initial sampling of $R = 20000$.

In conclusion, with a sampling of wavelengths at $R = 20000$, the thermal structure of red supergiant atmospheres is accurately computed, but there may be residual systematic errors in the sampled SED. So, that the spectrum is somewhat wrong does not mean that the thermal structure is! A better spectrum may be calculated using the computed atmospheric structure and a synthetic spectrum code. We will provide the detailed spectra either on the marcs.astro.uu.se or on the Pollux synthetic spectra database (Palacios et al. (2008); <http://pollux.graal.univ-montp2.fr>). Finally, remember that all this is within the adopted approximations of LTE, hydrostatic equilibrium, and spherical symmetry. Additional systematic errors are expected due to real stars not behaving in this simple way!

2. Affects of Velocity Fields on Spectra

Red supergiant atmospheres are strongly affected by convective motions, and large velocities have been measured through line shifts and broadening (e.g. Josselin & Plez 2007; Gray 2008a). Two types of non-thermal Doppler broadening must be taken into account: microturbulence and macroturbulence broadening. Both reflect our ignorance of real velocity fields in stellar atmospheres. Microturbulence was historically introduced to allow for a unique abundance when using strong and weak lines of the same species in spectroscopic analyses. Advocating some turbulent velocity field at a scale smaller than the photon mean free path, one can desaturate strong lines and increase their equivalent width at a given abundance. This was shown later to stem from convective motions in the case of the Sun, using sophisticated 3D hydrodynamical simulations (Asplund et al. 2000). Macroturbulence, a velocity field on a larger scale, may be necessary in addition to allow a fit of line widths, without impacting their equivalent width. Both microturbulent and macroturbulent velocities are most often assumed to follow a gaussian distribution. In the case of the Sun it was shown not to be correct: real lines are asymmetric. It is also the case for other stars, but we do not have as sophisticated models yet, nor the possibility to secure as detailed observations.

It is nevertheless very interesting to scrutinise a RSG spectrum to try to estimate the micro- and macroturbulent parameters. Fig. 1 and 2 show the detail of the $\text{TiO } \gamma' 0-0$ band-head in the spectrum of Betelgeuse (POP/ESO archive, Bagnulo et al. 2003). Model spectra were computed for appropriate parameters for α Ori (Levesque et al. 2005), and then convolved with different macroturbulent velocity distributions, all with a width of 15km/s: Gaussian, exponential, and radial-tangential (Gray 2008b). The radial-tangential distribution best fits the data, lending support to large granules rising in the atmosphere, with their upper layers moving horizontally before descending vertically again between the granules. Note that 15km/s is largely supersonic, which makes it difficult to advocate for such a turbulent velocity on small scales. The microturbulence velocity is not well constrained in RSGs but is quoted to be of the order of 2

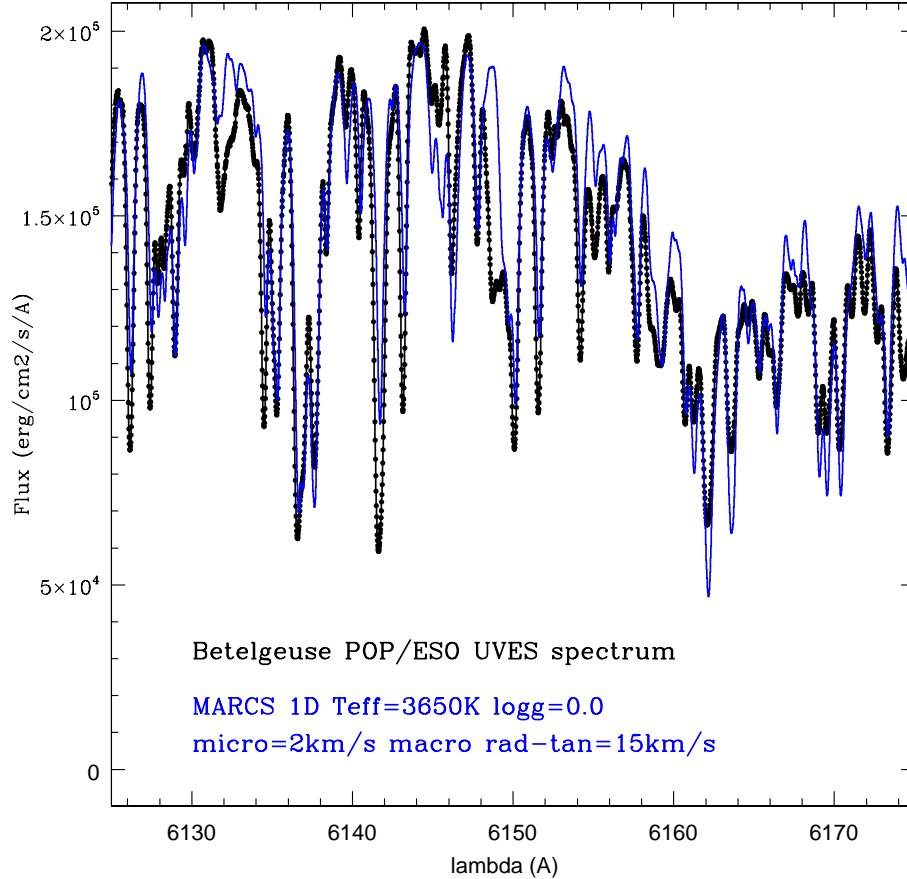


Figure 1. Comparison of a calculated spectrum (thin blue line) with a high resolution observed spectrum of Betelgeuse (black line with dots) in the vicinity of the γ' 0-0 band-head. Most spectral features are satisfactorily reproduced, although not perfectly. Considering the number of TiO lines present in this interval, most of which are not observed in the laboratory, and were predicted (Plez 1998), this is a very good fit. A microturbulence velocity of 2km/s and a radial-tangential macroturbulence of 15km/s were adopted.

to 6km/s (e.g. Carr et al. 2000; Luck & Bond 1989), with the high end values being supersonic! Line profile studies are impeded by line blending in cool supergiants. The IR region is clearly a better choice for such studies that should be intensified for a better understanding of RSG atmospheres.

2.1. Non-LTE effects in the formation of molecular lines

I give here a quick account of possible non-LTE effects in RSG atmospheres, summarising what was exposed in Plez (2008). TiO numerous electronic transition lines in the optical are a notorious cause of heating of the outer layers of cool stars. Surface heating or cooling only happens if the opacity is in absorption, and

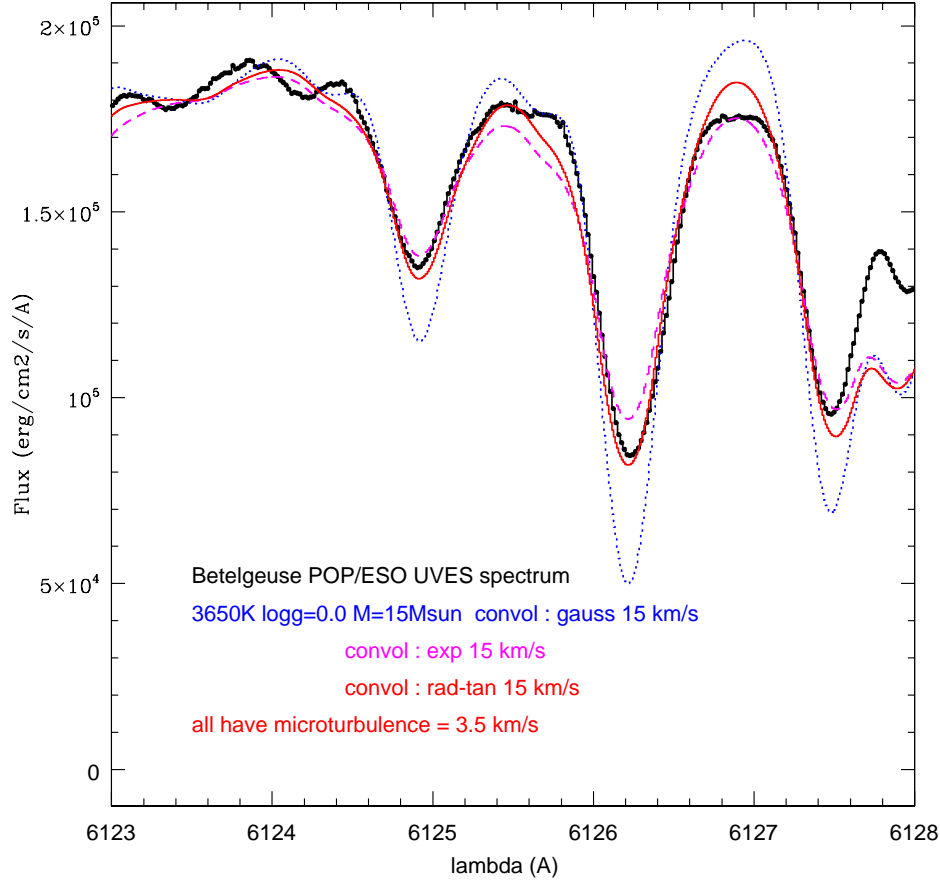


Figure 2. Impact of macro-turbulence on calculated spectra. High resolution observed spectrum of Betelgeuse (black line with dots) in the vicinity of the *gamma*' 0-0 band-head. A microturbulence velocity of 3.5km/s was adopted, and the spectrum is best matched setting a radial-tangential macro-turbulence of 15km/s (thin red line). Also shown are the effect of exponential 15km/s (magenta dashed line), and classical Gaussian 15km/s (blue dotted line) macro-turbulences.

scattering has no effect. It was suggested already by Hinkle & Lambert (1975) that some molecular lines do indeed form closer to scattering than pure absorption in the tenuous outer layers of red giants. Radiative rates for the optical and near IR TiO electronic transitions are of the order of $2.5 \times 10^7 s^{-1}$, whereas estimates in RSG atmospheric conditions lead to $2 \times 10^3 s^{-1}$ for collisions with electrons based on available recipes from van Regemorter (1962), and Jefferies (1968), and to $2 \times 10^6 s^{-1}$ for collisions with hydrogen, based on the modification by Lambert (1993) of the formula of Drawin (1969). Admittedly these approximations are far from justified for molecular transitions, and more theoretical and experimental work should be devoted to the determination of such collisional

rates [note the interesting work by Badie, J. M., Cassan, L. , & Granier, B. (2008) on quenching rates in YO]. Assuming radiative processes dominate over collisional ones in RSG atmospheres we may estimate the affect on the temperature structure. A large cooling indeed occurs in surface layers if TiO transitions are supposed to occur in scattering. This does not lead to large changes in the TiO band strengths themselves, but other lines are affected. Interestingly the cooling is what is required to allow observed $12\mu\text{m}$ H_2O lines to be reproduced (Ryde et al. 2006), but calculations with the cooled model do not show a good agreement with the $12\mu\text{m}$ spectrum, and OH lines become too strong. So, this simple way of modelling non-LTE effects in TiO transitions is not conclusive. A full NLTE treatment of the electronic transitions, taking into account optical depth effects, as the lines may become optically very thick, would be of great value. Also the coupling with hydrodynamics must be studied.

3. 3D Simulations of Red Supergiant Atmospheres

I have shown above, through selected examples that classical 1D, hydrostatic, and LTE model atmospheres, although leading to many successes (see e.g. Levesque et al. 2004), suffer limitations that have to be overcome. We know real stars are not 1D, static and in LTE! In particular in the case of RSGs, the hydrostatic approximation must be abandoned, and an hydrodynamical description used instead. This is not easy nor cheap however, as hydrodynamical equations, to be solved in 3D, must be coupled to the radiation field. There is an exchange of energy between the gas and the radiation field. Huge progress has been made in the past years, and we do have a small number of simulations for RSGs. These are star-in-a-box calculations made with the Co5bold code (Freytag et al. 2002). The whole star is put in the cartesian grid of the simulation volume, with an inner central boundary condition to avoid the nuclear burning core. The radiation field is described using a grey opacity. More details can be found in Freytag & Höfner (2008). Current simulations have up to 315^3 points, with $T_{\text{eff}} \approx 3500\text{K}$, $12M_{\odot}$, and a duration of a few years stellar time. Movies, and snapshots showing temperature, density, entropy, or velocity distributions can be found at <http://www.astro.uu.se/~bf/>. The simulation snapshots can be used to compute detailed polychromatic radiative transfer, which is by itself a very heavy task, and cannot be performed during the hydrodynamical calculations. This has been done by A. Chiavassa during his PhD thesis (Chiavassa 2008), available at <http://www.graal.univ-montp2.fr/hosted/chiavassa/publi.html>. The picture that emerge is that of a granulation with size a little smaller than the stellar radius, about as predicted by Schwarzschild (1975), velocities of tens of km/s (largely supersonic), and time-scales of months to years. The appearance of that granulation depends much on wavelength, with very great contrasts in the optical due to TiO absorption, and the strong dependency of the Planck function on temperature. The granulation is much less contrasted in the IR, but varies in aspect between the continuum and, e.g., strong CO lines. This results in a strong interferometric signal, both in visibility and phase, as shown by Chiavassa et al. (2008), that should allow a detailed characterisation of RSGs granulation pattern in a very near future. Interesting results on line profiles and asymmetries are already available. Fig. 3 shows an H_2O line as observed at 12.2

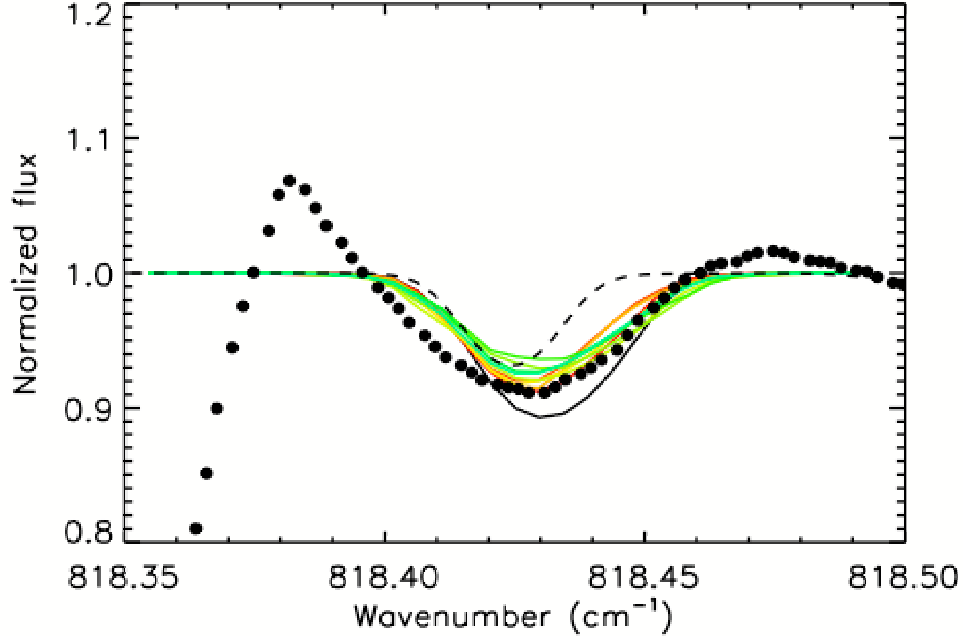


Figure 3. H₂O line near 12 μ m. Dots: TEXES observation (Ryde et al. 2006). Dashed line: MARCS 1D spectrum, with a microturbulence of 2km/s and an exponential macroturbulence of 13km/s. Thin lines: spectra for different snapshots from the same 3D simulation. The line broadening and shifts result from the velocity field generated by the simulation. No fudge micro- or macroturbulence are necessary.

drostatic MARCS model atmosphere, is far from matching the line strength or width, despite the use of ad'hoc micro- and macroturbulence velocities. The 3D calculations using the velocity field provided by the simulation do show shifts, and asymmetries that vary with time, and the line width is close to the observation, without the need for extra macroturbulence. This gives support to the radiative-hydrodynamical simulations. The agreement is not perfect though, as is also shown in Fig. 4 for an optical region of the spectrum in a TiO band. Lines appear slightly too narrow in the 3D simulated spectrum. The 1D MARCS spectrum does a better job, but at the price of two fudge parameters: a microturbulence and a macroturbulence velocity distributions (respectively gaussian and radial-tangential). So, the velocity dispersion of the 3D simulation seems a little too small, but is not very far from what is observed in RSGs. Inspection of larger chunks of spectra shows that the contrast of TiO bands is lower in the 3D model than in the corresponding 1D hydrostatic model. The explanation lies probably in the fact that the temperature gradient is too shallow in the 3D simulations. With a larger gradient in the line formation region, the contrast between strong and weak lines, or continuum would be greater.

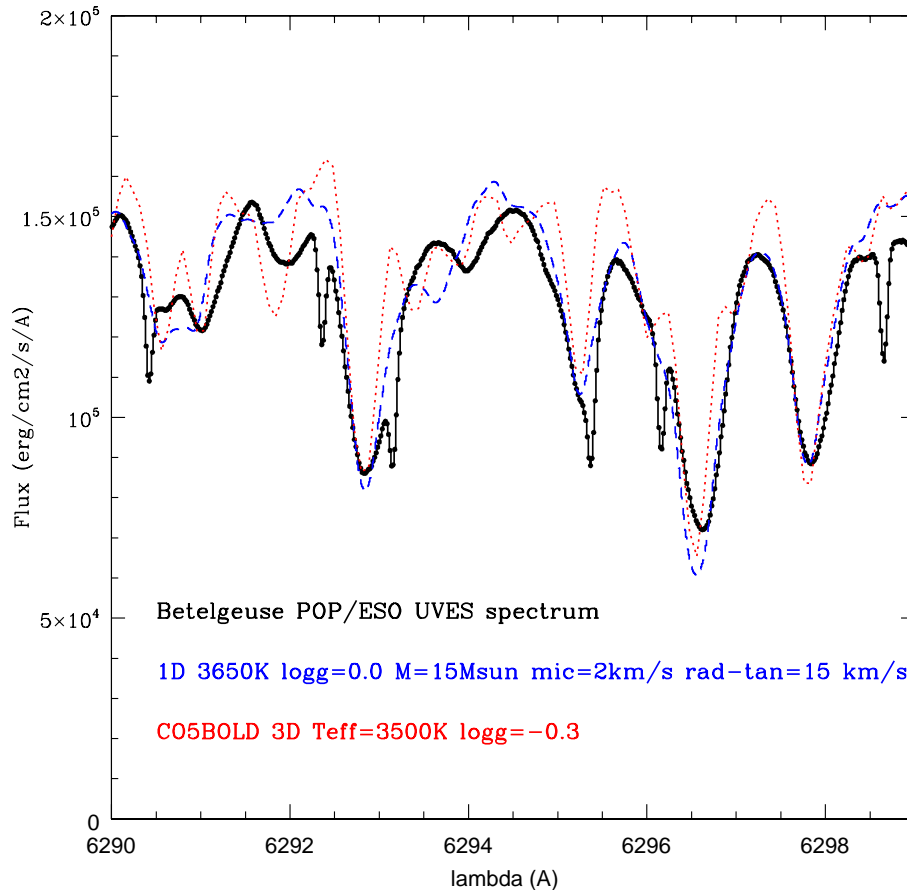


Figure 4. Detail of synthetic spectra for Betelgeuse. The thick black line with dots is the observed POP/UVES Betelgeuse spectrum. The blue dashed line is a MARCS 1D hydrostatic model spectrum with a microturbulence velocity of 2km/s and a 15km/s radial-tangential macroturbulence velocity distribution. The red dotted line is a Co5bold 3D hydrodynamical simulation snapshot spectrum, computed using the velocity field of the simulation. The adopted stellar parameters are slightly different but the main difference is in the velocity fields leading to line broadening : purely ad'hoc in the 1D case, and stemming from the radiative-hydrodynamical calculation in the 3D case.

4. Conclusions and Prospects

Classical 1D, LTE, hydrostatic model atmospheres are currently easily computed with a very detailed account of the wavelength dependence of opacity and radiation. They also include radiation pressure computed in detail at all depths. Input physical data, especially line data, is now adequate for the computation of cool stars, including RSGs. The drawback is that convection, and turbulent pressures are accounted through much too simple recipes. On the contrary the intricacy of 3D geometry with complicated velocity, temperature, and den-

sity distributions, certainly present in real RSGs, can only be described in 3D radiative-hydrodynamical simulations. This is of course possible only at the expense of simplifications in the treatment of the radiation field and related quantities, that are computed in the grey approximation (using Rosseland or Planck mean opacities). The 3D models do then predict velocity fields and temperature inhomogeneities, and detailed non-grey radiative transfer can be calculated a posteriori to produce images, and spectra. However, the velocity dispersion and the temperature gradient seem too shallow, when compared to observations. The models must be further developed, in particular with a non-grey radiative transfer, based on a small number of opacity bins, the only tractable solution for now. This should lead to greater temperature gradients. The inclusion of radiative pressure could help increase velocity fields to the observed levels. Once these 3D models are in a satisfactory state, validated by observations, we should devise recipes that can be incorporated in easier to compute, and manipulate, 1D (or 2D) models.

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